

# Superfluidity of Bosons in Kagome Lattices with Frustration

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In this letter we consider spinless bosons in Kagome lattice with nearest-neighbor hopping and on-site interaction, and the sign of hopping is inverted by inseting a  $\pi$  flux in each triangle of Kagome lattice so that the lowest single particle band is perfectly flat. We show that in the high density limit, despite of the infinite degenerate of the single particle ground state, interaction will select out the Bloch state at the  $K$  point of Brillouin zone for boson condensation at the lowest temperature. As temperature increases, we show that the single boson superfluid order can be easily destroyed, while an exotic triple-boson paired superfluid order will remain. This trion superfluid exist in a broad temperature window until the temperature is increased to the same order of hopping and then the system turns into normal phases. Finally we show that time-of-flight measurement of momentum distribution can be used to distinguish these three phases.

Flat band models have attracted considerable theoretical interests recently [1–13], because the single particle energies are degenerate inside the flat band, therefore interactions play a dominative role in the many-body system and lead to many interesting quantum phases [7–13]. Among many different physical realizations of lattice models with flat band, Kagome lattices with only nearest neighbor hopping is perhaps one of the simplest. Recently, such a model has been realized experimentally using optical lattices by the Berkeley group [14]. However, the flat band in a normal Kagome lattice is the highest band. By fast shaking the optical lattices, one can invert the sign of hopping, which has also been demonstrated experimentally for triangular optical lattices [15]. This technique can be applied straightforwardly to Kagome lattices. When the sign of hopping is inverted, it is equivalent to inseting a  $\pi$  flux in each triangle of the Kagome lattice, and the flat band becomes the lowest band, as shown in Fig. 1. Thus, the kinetic energy is frustrated on such a Kagome lattice.

In this letter we consider spinless bosons with on-site interaction on the Kagome lattice with frustration, and we focus on the high density limit, where the system is away from strongly correlated phases like Mott insulator[7, 8], Wigner crystal[9] and quantum Hall state[10, 11]. This high density limit corresponds to a real system with a Kagome optical lattice in the  $xy$  plane and weak confinement potential along the  $\hat{z}$  direction. Therefore, each site is in fact a tube inside which bosons form a quasi-condensate, and tunneling couples different tubes that leads to a two-dimensional Josephson array described by a two-dimensional boson Hubbard model.

Here we shall discuss whether and how bosons can condense in the flatband, and what exotic type of superfluid occurs at finite temperature. The main findings are

(1) Though the lowest band of the single particle state is infinitely degenerate, interaction will select out a unique single particle state for bosons to condense at the lowest temperature. We show that this unique single particle state is the Bloch state at the  $K$  point.

(2) As temperature increases, the single boson superfluid order can be easily destroyed. However, a triple-boson paired superfluid order will remain until the temperature is of the order of hopping energy and the system turns into normal. Thus we predict a large temperature window in which the system has an exotic “trion superfluid” phase.

(3) We show that a simple time-of-flight (TOF) detection of momentum distribution can distinguish  $K$  point conventional condensate, trion condensate and normal phase.

It has been a long term efforts to search exotic bosonic state that has no single-boson superfluid order. In previous studies, two-boson paired superfluids (or charge-4e superconductor as paired Cooper pairs) have been proposed in various systems, such as stripe superconductor [17], FFLO superconductor [18–20], spin-1 bosons [21–24] and bosons with Rashba spin-orbit coupling [25]. These boson paired superfluid phase emerges from melting of stripe order or internal spin order. But none of them have been observed yet. As far as we know, it is the first time that a triple-boson paired superfluid is proposed, and the underlying physical mechanics, that is, the kinetic energy frustration due to the particular Kagome geometry, is also different from that of previous examples. These results may also be generalized to interacting bosons in other flat band models with geometric frustration.

**Band Structure and Mean-Field.** The boson Hubbard model on the Kagome lattice with  $\pi$  flux in each triangle is given by  $\hat{H} = \hat{H}_t + \hat{H}_U$ , with the hopping term  $\hat{H}_t = t \sum_{\langle ij \rangle} \hat{b}_i^\dagger \hat{b}_j + h.c.$ , and the interaction term  $\hat{H}_U = U \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$ , where  $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ . Here  $t$  is positive [16]. In the momentum space, the hopping Hamiltonian reads  $\hat{H}_t = \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger h(\mathbf{k}) \hat{b}_{\mathbf{k}}$  with  $\hat{b}_{\mathbf{k}} = (\hat{b}_{\mathbf{kA}}, \hat{b}_{\mathbf{kB}}, \hat{b}_{\mathbf{kC}})^\top$  and

$$h(\mathbf{k}) = 2t \begin{pmatrix} 0 & \cos k_3 & \cos k_2 \\ \cos k_3 & 0 & \cos k_1 \\ \cos k_2 & \cos k_1 & 0 \end{pmatrix}, \quad (1)$$

where  $k_i \equiv \mathbf{k} \cdot \mathbf{a}_i$ , and  $\mathbf{a}_1 = (1, 0)$ ,  $\mathbf{a}_2 = (-\frac{1}{2}, \frac{\sqrt{3}}{2})$ ,

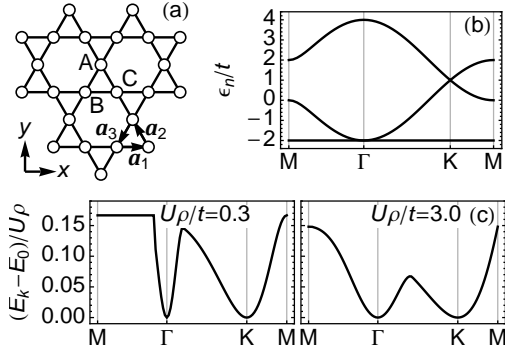


FIG. 1: (a) Kagome lattice, partitioned into A, B, C sublattices. (b) Band structure with inverted hopping sign, where  $\Gamma = (0, 0)$ ,  $K = (2\pi/3, 0)$  and  $M = (\pi/2, \pi/2\sqrt{3})$ . (c) Mean field energy landscape for different  $U\rho/t$ . Energy shifted by  $E_0 = -2t + U\rho/3$  ( $\rho$  = the boson density per unit cell).

$\mathbf{a}_3 = (-\frac{1}{2}, -\frac{\sqrt{3}}{2})$  as shown in Fig. 1(a). The band structure contains three bands: two are dispersive, and one is flat. The flat band is the lowest band, with a quadratic touching point between the lowest and the first excited band at  $\Gamma$  point, as shown in the Fig. 1(b).

Because of the infinite degeneracy of the single particle ground state, bosons can not condense if there is no interaction. However, once the interaction energy is included, the single particle degeneracy will be lifted. Here we shall first discuss how the interaction select out a unique single particle state for boson condensation. At the mean-field level, we first consider the single particle state with translational symmetry labelled by momentum  $\mathbf{k}$ . Taking the mean-field ansatz  $\langle b_{\mathbf{k}} \rangle = z \equiv (z_A, z_B, z_C)^T$  with the normalization condition  $z^\dagger z = \rho$ , where  $\rho$  is the boson filling per unit cell, we can minimize the whole mean-field energy function  $E_{\mathbf{k}}[z] = z^\dagger h(\mathbf{k})z + U(|z_A|^4 + |z_B|^4 + |z_C|^4)$  with respect to  $z$ , and denote the optimal mean field energy as  $E_{\mathbf{k}} = \min_z E_{\mathbf{k}}[z]$ . This mean field energy landscape is shown in Fig. 1(c).

Fig. 1(c) shows that the single particle degeneracy is lifted by the Hartree energy. This is because inside the flat band, only the single particle wave function of the  $K$  point has equal amplitude in three sublattices, and therefore only at  $K$  point the density is uniform and the repulsive interaction energy is the smallest. While nearby  $\Gamma$  point, a uniform density state can be achieved by forming a superposition between the lowest and the first excited band, and such a superposition costs no energy at  $\Gamma$  point because of the quadratic band touching. Thus, the mean-field energy select out the  $\Gamma$  and  $K$  points.

The Bloch wave function for  $\Gamma$  and  $K$  points determined by mean-field energy read

$$\begin{aligned} \psi_{\Gamma}(\mathbf{r}_i) &= \frac{1}{\sqrt{3}}(1, e^{\pm 2\pi i/3}, e^{\mp 2\pi i/3})^T, \\ \psi_K(\mathbf{r}_i) &= \frac{1}{\sqrt{3}}e^{i\mathbf{k}_K \cdot \mathbf{r}_i}(1, -1, -1)^T, \end{aligned} \quad (2)$$

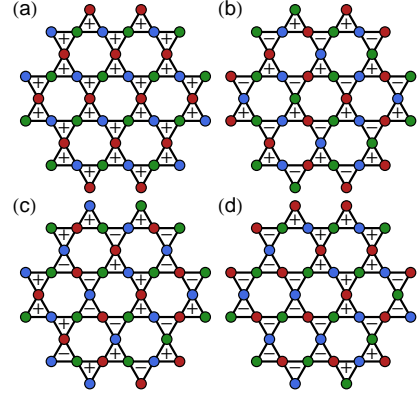


FIG. 2: (Color online.) (a-b) Phase configuration of the condensate at  $\Gamma$  point (a) and  $K$  point (b), (c-d) random 3-color arrangement. Phases are denoted by colors: red = 1, green =  $e^{2\pi i/3}$ , blue =  $e^{4\pi i/3}$ . “ $\pm$ ” mark out the vorticity around each triangle.

with  $\mathbf{k}_K = (2\pi/3, 0)$ . In the real space, both two wave functions satisfy two conditions: (i) their densities are uniform, which minimize the mean-field interaction energy and (ii) their phases follow “3-color arrangement”. Here “3-color arrangement” means that each pair of two neighboring sites take different phases out of 1,  $e^{2\pi i/3}$  and  $e^{-2\pi i/3}$ , as depicted in Fig. 2. It is easy to show that once the “3-color arrangement” is satisfied, the kinetic energy is also minimized. “3-color arrangement” requires that three sublattices in each triangle must all take different phases, and one can define “vorticity” for each triangle. Vorticity  $+$ ( $-$ ) means that the phase increases clockwise (anti-clockwise). As shown in Fig. 2(a) and (b),  $\psi_{\Gamma}$  is a “vorticity ferromagnetic” state and  $\psi_K$  is a “vorticity antiferromagnetic” state.

In fact, once above condition (i) and (ii) are satisfied, both kinetic and interaction energy are simultaneously minimized at the mean-field level. The translation invariance is not a necessary condition and can be released. In fact, one can find extensive number of states without translation invariance that satisfies both (i) and (ii), and two of such examples are depicted in Fig. 2(c-d). These states are locally identical to either  $K$  state or  $\Gamma$  state, and the domain wall costs no energy at mean-field level.

*Quantum Fluctuation and Order from Disorder.* These extensive number of degenerate mean-field states can be further lifted by quantum fluctuations, because the zero-point energy of Bogoliubov phonons is different for different mean-field state. For a given mean-field configuration  $\langle \hat{b}_i \rangle = z_i$ , its Bogoliubov Hamiltonian is

$$\begin{aligned} H[z_i] &= t \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + h.c.) - \mu \sum_i \hat{b}_i^\dagger \hat{b}_i \\ &\quad + U \sum_i \left( 2|z_i|^2 \hat{b}_i^\dagger \hat{b}_i + z_i^2 \hat{b}_i^\dagger \hat{b}_i^\dagger + h.c. \right), \end{aligned} \quad (3)$$

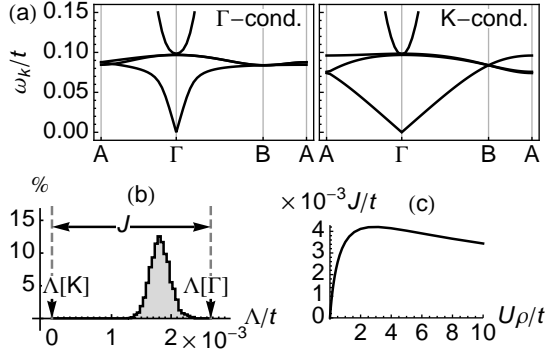


FIG. 3: (a) Bogoliubov spectra for  $\Gamma$  point (left) and  $K$  point (right) condensates at  $U\rho/t = 0.3$ . Momentum points are defined as  $A = (\pi/3, 0)$  and  $B = (\pi/3, \pi/3\sqrt{3})$ . (b) Distribution of the zero point energies of all degenerate mean-field configurations. The horizontal axes are zero-point energy  $\Lambda$  of degenerate mean-field state, and two dashed lines denote the zero-point energy for  $K$  and  $\Gamma$  point condensate. The vertical axes is the probability for having this zero-point energy. (c)  $J/t$  v.s.  $U\rho/t$  plot.

where  $\mu = -2t + 2U\rho/3$ . Diagonalization of  $H[z_i]$  leads to  $H[z_i] = \sum_m \omega_m[z_i] (\hat{\gamma}_m^\dagger \hat{\gamma}_m + 1/2)$ , with  $\hat{\gamma}_m$  being Bogoliubov boson operator. Thus the vacuum energy associated with this given condensate configuration equals to  $\Lambda[z_i] = \frac{1}{2} \sum_m \omega_m[z_i]$  by setting  $\hat{\gamma}_m^\dagger \hat{\gamma}_m = 0$ .

For condensates at  $\Gamma$  and  $K$  points, the Bogoliubov excitations have quantum number  $\mathbf{k}$  and they have well defined dispersion as shown in Fig. 3(a). One finds that the sound velocity  $c$  of  $K$  point condensate is smaller than that of  $\Gamma$  point condensate. This is also evidenced from the mean field energy landscape as shown in Fig. 1(c), where energy landscape changes less rapidly nearby  $K$  point than that nearby  $\Gamma$  point, indicating softer Goldstone mode and more quantum fluctuations. Roughly speaking, the zero point energy is proportional to the sound velocity squared, i.e.  $\Lambda \sim c^2$ , the degeneracy between  $\Gamma$  point and  $K$  point configurations will thus be lifted by their different zero point energies.

For a generic mean-field state in the degenerate manifold, the Bogoliubov spectrum has no well defined dispersion because of the absence of translation symmetry. Here we randomly sample over 4000 configurations on a 240-site Kagome lattice which have uniform density and satisfy “3-color arrangement”, and then calculate their zero-point energy numerically. We find that their zero-point energies all rest between  $\Gamma$  point condensate and  $K$  point condensate, i.e.  $\forall \{z_i\} : \Lambda[K] \leq \Lambda[z_i] \leq \Lambda[\Gamma]$ , as seen from Fig. 3(b). Now the degeneracy has been completely removed through the order-by-disorder mechanism. At sufficient low temperature, bosons will condense to  $K$  point (or its symmetry related points).

*Thermal Fluctuation and Phase Diagram.* We have mentioned that all mean-field degenerate states can be

locally viewed as either  $K$ -point or  $\Gamma$  point, it is natural to introduce an energy scale  $J = \Lambda[\Gamma] - \Lambda[K]$  as the typical energy cost for creating domain walls, which entirely comes from the fluctuation energy. As shown in Fig. 3(c),  $J$  will vanish in both small and large  $U\rho$  limit. The asymptotic behavior goes like  $J \propto U\rho$  for  $U\rho \ll t$  and  $J \propto t^{3/2}(U\rho)^{-1/2}$  for  $U\rho \gg t$ . The maximum of  $J$  is achieved around  $U\rho/t = 3$  which is of the order  $10^{-3}t$ . It is still quite challenging to reach such low temperature for current cold atom experiment.

However, in contrast to many systems, at the lowest temperature the system is a conventional Bose condensate which by itself is not the most interesting phase. The most interesting phase in this system exists at the temperature regime  $k_B T > J$ . In this regime, the domain wall will proliferate and the system will enter a thermal mixed state in which all mean-field configurations satisfying condition (i) and (ii) mentioned above are almost equally populated. In this thermal mixed state, for each site the condensate phase can take  $\theta_i = 0, \pm 2\pi/3$  with equal probabilities. Thus, the single boson correlation will become short-ranged, i.e.  $\langle \hat{b}_i^\dagger \hat{b}_j \rangle = \rho_s \langle e^{-i\theta_i} e^{i\theta_j} \rangle \rightarrow 0$ . However, we notice that as long as the “3-color arrangement” is satisfied, at every site  $e^{3i\theta_i} \equiv 1$  is always hold. Thus, the triple bosons operator can still possess long-range correlation, i.e.  $\langle \hat{b}_i^\dagger \hat{b}_j^3 \rangle = \rho_s^3 \langle e^{-3i\theta_i} e^{3i\theta_j} \rangle \rightarrow \rho_s^3$ . Since the “3-color arrangement” is enforced by the kinetic energy, thus, it will not be destroyed by thermal fluctuations as long as  $T < t$ . Therefore we propose that within the temperature range  $J < T < t$ , there will be a “trion superfluid” phase in which the bosons condense in triples. This trion superfluid supports many interesting properties, such as  $1/3$  fractionalized vortices, which will be studied in the future.

When temperature is increased to the same order of  $t$ , the “3-color arrangement” will be destroyed, and the long wave-length fluctuation of the  $U(1)$  phase will lead to a Kosterlitz-Thouless phase transition from the “trion superfluid” to the normal state. This transition temperature can be estimated from the superfluid stiffness, which can be calculated from the free energy response to the phase twist. Let  $b_i = w_i e^{i\theta_i} e^{i\mathbf{q} \cdot \mathbf{r}_i}$ , where  $e^{i\mathbf{q} \cdot \mathbf{r}_i}$  is the applied phase twist. In the temperature regime  $T \gg J$ , we can ignore the zero-point energy, and the energy functional for a given  $\{\theta_i\}$  configuration reads  $E_{\mathbf{q}}[\theta_i, w_i] = t \sum_{\langle ij \rangle} (w_i^* w_j e^{-i(\theta_i - \theta_j)} e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} + h.c.) + U \sum_i |w_i|^4$ , and because all the configurations must be taken into account under thermal average, the averaged energy functional reads

$$\begin{aligned} \mathcal{E}_{\mathbf{q}}[w_i] &= \sum_{\{\theta_i\}} E_{\mathbf{q}}[\theta_i, w_i] \\ &= -\frac{t}{2} \sum_{\langle ij \rangle} (w_i^* w_j e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} + h.c.) + U \sum_i |w_i|^4 \quad (4) \end{aligned}$$

It is interesting to note that Eq. (4) is the same of a

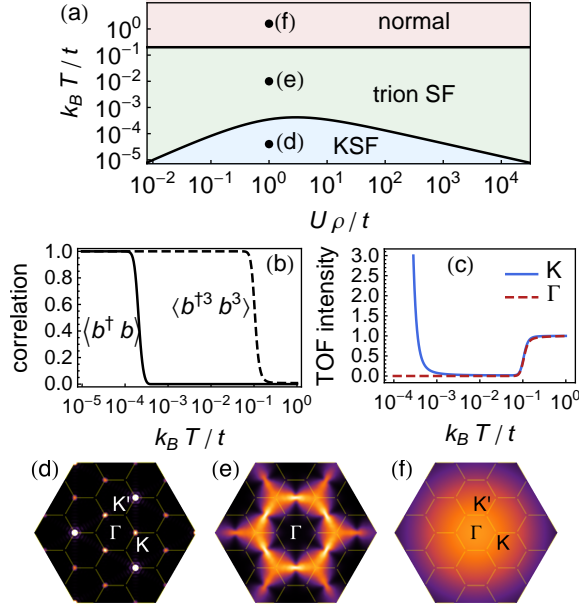


FIG. 4: (Color on line.) (a) Phase diagram. It contains three phases: the conventional superfluid phase with boson condensation at  $K$  point (KSF), three-boson paired (trion) superfluid (Trion SF) phase, and the thermal gas phase. (b) The long-range correlation for  $\langle b^\dagger b \rangle$  and  $\langle \hat{b}_i^\dagger \hat{b}_j^3 \rangle$  as a function of temperature  $k_B T/t$ . (c) Time-of-flight intensity at  $\Gamma$  and  $K$  point as a function of temperature  $k_B T/t$ . (d-f): Time-of-flight image of momentum distribution for three typical points in the phase diagram (a). Brighter color indicates larger boson density. The thin line of honeycomb marks out the Brillouin zone. For (b-f), we have set  $U\rho/t = 1$ .

mean-field energy of bosons in the Kagome lattice *without* frustration, because the sign of hopping is now inverted back. Mathematically, it is because taking thermal average leads to  $\langle e^{i(\theta_i - \theta_j)} \rangle = -1/2$ . Physically, it can be elaborated more clearly by a fractionalization representation [26]. Since the kinetic energy frustration is released, trion superfluid will have a finite stiffness. It can be obtained by minimizing  $\mathcal{E}_q[w_i]$  with respect to  $w_i$  and expand the optimal energy in terms of small  $q$ , which leads to  $\min_{\{w_i\}} \mathcal{E}_q[w_i] \simeq -2t + \frac{U\rho}{3} + \frac{1}{2}tq^2$ . Therefore, the stiffness is  $t$ , which gives an estimate of the Kosterlitz-Thouless transition temperature as  $T_{KT} = t/\pi$ .

With the analysis above, we reach the phase diagram as shown in Fig. 4(a). In Fig. 4(b), we show the one-boson and three-boson correlation function as a function of temperature for a fixed  $U\rho/t$ . The one-particle correlation  $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$  is calculated as  $\rho_s \sum_{\{\theta_i\}} e^{-i(\theta_i - \theta_j)} e^{-\Lambda[\theta_i]/T}$ . Because we expect this correlation vanishes at very low temperature of the order  $J$ , we can restrict the summation to the configurations that satisfy the “3-color arrangement” since other configuration cost energy of the order  $t$  and their contribution is negligible in low temperature.  $\Lambda[\theta_i]$  is the zero point energy of each condensate.

While on the other hand, when we calculate the three-boson correlation  $\langle \hat{b}_i^\dagger \hat{b}_j^3 \rangle = \rho_s^3 \sum_{\{\theta_i\}} e^{-3i(\theta_i - \theta_j)} e^{-E[\theta_i]/T}$ , the summation goes over all configurations  $\{\theta_i\}$ , and the energy is given by  $E[\theta_i] = 2t \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$ , where we have ignored the zero-point energy since  $\Lambda[\theta_i]$  is negligible compared to  $E[\theta_i]$ . Fig. 4(b) shows that there indeed exists a large temperature window there the one-boson correlation function vanishes while the three-boson correlation function remains finite.

*Detection.* Finally we show that the difference between these three phases can be detected by a straightforward measurement of momentum distribution via TOF image. When bosons condense into  $K$  points of the Brillouin zone, TOF image will display sharp Bragg peaks at  $K$  point (or its equivalent  $K'$  point) and its reciprocal lattice vector, as shown in Fig. 4(d). Moreover, due to the interference effect from the phase structure satisfying the “3-color-arrangement”, it is easy to show that the strongest peaks do not appear in the first Brillouin zone, but instead at its reciprocal lattice points in the second Brillouin zone. As temperature increases to the trion superfluid phase, all the 3-color arrangements are thermally mixed, and the Bragg peak at  $K$  point disappears as the single-boson superfluid order vanishes. However, in contrast to normal state, the TOF image is not featureless. In fact, a large honeycomb structure appears and the hexagon is 4 times of the area of the first Brillouin zone, as shown in Fig. 4(e). The intensity at  $\Gamma$  point is always zero, because for zero-momentum component of the Fourier transformation is exactly cancelled out due to the “3-color arrangement”. At the highest temperature normal state, the TOF image becomes a featureless Gaussian and the intensity at  $\Gamma$  point becomes the maximum, as shown in Fig. 4(f). Thus, we predict that the intensity at  $K$  point rapidly decreases at the transition from conventional  $K$ -point condensate to trion superfluid, and the intensity of  $\Gamma$  point rapidly increases at the transition from trion superfluid to normal state, as shown in Fig. 4(c). Besides, the trion superfluid order can be also probed by the 3-point correlation function of the TOF image.

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